Discrete Multiscale Modelling and Future Research Plans concerning Metals

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The quasicontinuum (QC) method [1] is multiscale approach that coarse-grains discrete models in regions with slowly fluctuating and fully resolves the discrete model in regions where individual small-scale mechanics need to be captured. It is mainly used for conservative atomistics, but has recently been formulated based on a virtual-power statement, allowing the method to be used for a wide variety of applications that include dissipation [2]. Examples are bond sliding in paper materials [3] and electronic textile [4].

Besides an overview of the virtual-power-based QC method, this presentation will also give examples in which the QC method is used for FCC crystals [5] and future plans to use the approach for open-cell metal foams with functionally graded coatings. An introduction in other future research plans of the authors, not related to QC approaches, is also given and deal with (i) using XFEM to resolve discretisation issues in crystal plasticity, (ii) the development of a multitime approach to reduce the computational costs of low cycle fatigue and (iii) Fast-Fourier-Transformation of periodic representative volume elements.

[1] Tadmor EB, Ortiz M, Philips R, *Quasicontinuum analysis of defects in solids*, Phil. Mag. A, 73 (1996) 1529-1563.
[2] Beex LAA, Peerlings RHJ, Geers MGD, *A multiscale quasicontinuum method for dissipative lattice models and discrete networks*, J. Mech. Phys. Solids., 64 (2014) 154-169.
[3] Beex LAA, Peerlings RHJ, Geers MGD, *A multiscale quasicontinuum method for lattice models with bond failure and fiber sliding*, Comput. Meth. Applied M., 269 (2014) 108-122.
[4] Beex LAA, Peerlings RHJ, Van Os K, Geers MGD, *The mechanical reliability of an electronic textile investigated using the virtual-power-based quasicontinuum method*, Mech. Mater., DOI: 10.1016/j.mechmat.2014.08.001.
[5] Beex LAA, Peerlings RHJ, Geers MGD, *Central summation in the quasicontinuum method*, J. Mech. Phys. Solids., 70 (2014) 242-261.